The Boltzmann Equation

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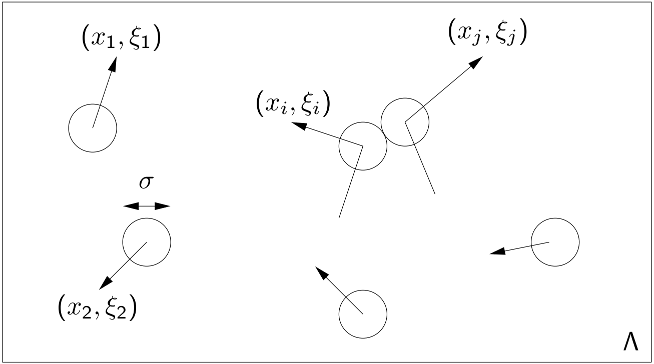
Outline

Outline

The Hard Sphere Model of a Gas



- Particles are modeled as solid spheres wth diameter σ.
- Dynamical features are linear movement and collisions among particles
- We will work with periodic boundary conditions ($\Rightarrow$ no collisions with $\partial\Lambda$)
- The state of each particle is given by its position x_i and its velocity ξ_i.
- The state of the system is given as a point $z^N = (x_1, \xi_1 \ldots x_N, \xi_N)$ in the phase space $\Gamma = \{z^N \in \Lambda^N \times \mathbb{R}^{3N}; |x_i - x_j| \geq \sigma \text{ for } i \neq j\}$

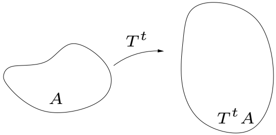
Probability distribution functions

- Number of particles $N \sim \mathcal{O}(10^{23}) \Longrightarrow$ For practical purposes we use a probability density function $P(z^N, t) = P(x_1, \xi_1, \ldots, x_N, \xi_N, t)$, $P(z^N, t) \in L^1(\Gamma)$.
- Essential property:

$$P(\ldots x_i, \xi_i \ldots x_j, \xi_j \ldots, t) = P(\ldots x_j, \xi_j \ldots x_i, \xi_i \ldots, t)$$

- Let $T^t : \Gamma \to \Gamma$ describe the time evolution of the system. We have for all Borel sets A:

$$\int_A P(z^N, 0)\, dz^N = \int_{T^t A} P(T^t z^N, t)\, d(T^t z^N) = \int_A P(T^t z^N, t) \left| \frac{\partial T^t z^N}{\partial z^N} \right| dz^N$$



- We will now prove that $\left| \frac{\partial T^t z^N}{\partial z^N} \right| = 1$.

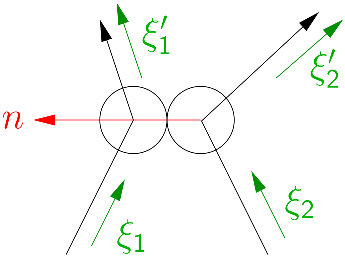
The Jacobian of the time evolution

- Between collisions: $x'_i = x_i + \xi_i t$, $\xi'_i = \xi_i$, so

$$\left| \frac{\partial(x'_i, \xi'_i)}{\partial(x_j, \xi_j)} \right|_{\text{no collision}} = \delta_{ij} \left| \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \right| = 1$$

- At collision points: $x'_i = x_i$, $\xi'_i \neq \xi_i$, so

$$\frac{\partial x'_i}{\partial x_j} = \delta_{ij} \; ; \quad \frac{\partial x'_i}{\partial \xi_j} = 0 \quad \text{for } 1 \leq i, j \leq N.$$



The Jacobian of the time evolution

- At collision points we have:

$$\begin{aligned} \xi_1 + \xi_2 &= \xi_1' + \xi_2' && \text{Momentum conservation} \\ |\xi_1|^2 + |\xi_2|^2 &= |\xi_1'|^2 + |\xi_2'|^2 && \text{Energy conservation} \end{aligned}$$

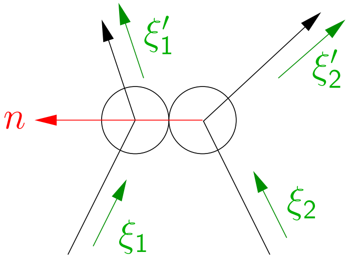
- It follows that

$$\begin{aligned} \xi'_{1\alpha} &= \xi_{1\alpha} - n_\alpha [n_\beta \cdot (\xi_{1\beta} - \xi_{2\beta})] \\ \xi'_{2\alpha} &= \xi_{2\alpha} + n_\alpha [n_\beta \cdot (\xi_{1\beta} - \xi_{2\beta})] \end{aligned}$$

where $n = (x_1 - x_2)/|x_1 - x_2|$. So

$$\frac{\partial \xi'_{1\alpha}}{\partial \xi_{1\beta}} = \delta_{\alpha\beta} - n_\alpha n_\beta$$

$$\frac{\partial \xi'_{1\alpha}}{\partial \xi_{2\beta}} = n_\alpha n_\beta$$



The Jacobian of the time evolution

- Putting the pieces together:

$$
\begin{aligned}
\left|\frac{\partial(x_i', \xi_i')}{\partial(x_j, \xi_j)}\right|_{\text{collision}}
&= \begin{vmatrix}
\begin{matrix} \frac{\partial x_1}{\partial x_1} & \frac{\partial x_1}{\partial x_2} \\ \frac{\partial x_2}{\partial x_1} & \frac{\partial x_2}{\partial x_2} \end{matrix} & \frac{\partial \xi_{1/2}}{\partial x_{1/2}} \\
\frac{\partial x_{1/2}}{\partial \xi_{1/2}} & \begin{matrix} \frac{\partial \xi_1}{\partial \xi_1} & \frac{\partial \xi_1}{\partial \xi_2} \\ \frac{\partial \xi_2}{\partial \xi_1} & \frac{\partial \xi_2}{\partial \xi_2} \end{matrix}
\end{vmatrix} \\
&= \begin{vmatrix}
\begin{matrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{matrix} & * \\
0 & \begin{matrix} \mathbb{1} - nn^T & nn^T \\ nn^T & \mathbb{1} - nn^T \end{matrix}
\end{vmatrix} \\
&= 1
\end{aligned}
$$

- Several (distinct) collisions at the same time do not change this result.
- The following sets have zero measure and can be neglected:
  - Configurations leading to collisions that involve 3 or more particles.
  - Configurations leading to infinitely many collisions in a finite time.

(Proof: Cercignati, Illner, Pulvirenti: The Mathematical theory of Dilute Gases, Springer 1994)

The Liouville Equation

- We had

$$\int_A P(z^N, 0) = \int_A P(T^t z^N, t) \underbrace{\left| \frac{\partial T^t z^N}{\partial z^N} \right|}_{=1} dz^N$$

- As A was arbitrary, we obtain the Liouville Equation

Theorem (Liouville Equation)

For a hard sphere system with a measurable probability density function P the following equation holds:

$$\frac{d}{dt} P(T^t z^N, t) = 0 \quad \text{for almost all } z^N$$

- For smooth P this reduces to

$$\frac{\partial P}{\partial t} + \sum_{i=1}^{N} \xi_i \frac{\partial P}{\partial x_i} = 0$$

The s-particle distribution function

- The N-particle distribution P is not of much practical use. Therefore we define the s-particle distribution function

$$P^{(s)}(x_1, \xi_1, \ldots, x_s, \xi_s, t) = \int P(x_1, \xi_1, \ldots, x_N, \xi_N) \prod_{j=s+1}^{N} dx_j d\xi_j$$

  It gives the probability of finding s preselected particles in a configuration $(x_1, \xi_1 \ldots x_s, \xi_s)$, leaving the parameters of the other particles arbitrary.
- We will now derive a relation between $P^{(s)}$ and $P^{(s+1)}$.
- For smooth P, the Liouville equation $\frac{\partial P}{\partial t} + \sum_{i=1}^{N} \xi_i \frac{\partial P}{\partial x_i}$ =0 yields

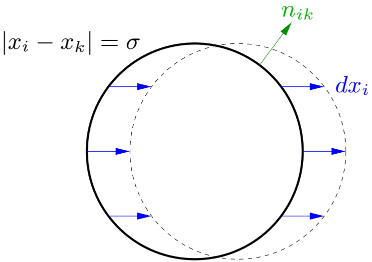
$$\begin{aligned} \frac{\partial P^{(s)}}{\partial t} &+ \sum_{i=1}^{s} \int \xi_i \frac{\partial P}{\partial x_i} \prod_{j=s+1}^{N} dx_j d\xi_j \\ &+ \sum_{k=s+1}^{N} \int \xi_k \frac{\partial P}{\partial x_k} \prod_{j=s+1}^{N} dx_j d\xi_j = 0 \end{aligned}$$

Derivation of the BBGKY Hierarchy

- First integral:

$$\sum_{i=1}^{s} \int \xi_i \frac{\partial P}{\partial x_i} \prod_{j=s+1}^{N} dx_j d\xi_j = \sum_{i=1}^{s} \xi_i \frac{\partial P^{(s)}}{\partial x_i} - \sum_{i=1}^{s} \sum_{k=s+1}^{N} \int P^{(s+1)} \xi_i \cdot n_{ik} d\sigma_{ik} d\xi_k$$

$d\sigma_{ik}$	=	surface element of the sphere $\lvert x_i - x_k \rvert = \sigma$ around x_k
n_{ik}	=	Outer normal to this sphere
$P^{(s+1)}$	=	$P^{(s+1)}(x_1, \xi_1 \ldots x_s, \xi_s, x_i - n_{ik}\sigma, \xi_k, t)$



Derivation of the BBGKY Hierarchy

- The second integral can be solved using the Gauss theorem:

$$\sum_{k=s+1}^{N} \int \xi_k \frac{\partial P}{\partial x_k} \prod_{j=s+1}^{N} dx_j d\xi_j =$$

$$\sum_{k=s+1}^{N} \sum_{i=1}^{s} \int P^{(s+1)} \xi_k \cdot n_{ik} d\sigma_{ik} d\xi_k + \sum_{\substack{i,k=s+1 \\ i \neq k}}^{N} \int P^{(s+2)} \xi_k \cdot n_{ik} d\sigma_{ik} d\xi_k dx_i d\xi_i =$$

$$\sum_{k=s+1}^{N} \sum_{i=1}^{s} \int P^{(s+1)} \xi_{s+1} \cdot n_i d\sigma_i d\xi_{s+1} - \frac{1}{2} \sum_{\substack{i,k=s+1 \\ i \neq k}}^{N} \int P^{(s+2)} \cdot \underbrace{(\xi_i - \xi_k)}_{=:V_{ik}} \cdot n_{ik} d\sigma_{ik} d\xi_k dx_i d\xi_i$$

- At collisions, each point on the hemisphere $V_{ik} \cdot n_{ik} > 0$ correspondes to a point on $V_{ik} \cdot n_{ik} < 0$:

$$P^{(s+2)}(\ldots x_i, \xi_i, x_k, \xi_k, t) = P^{(s+2)}(\ldots x_i, \xi_i - n_{ik}(n_{ik} V_{ik}), x_k, \xi_k + n_{ik}(n_{ik} V_{ik}), t)$$

- Therefore, $\int P^{(s+2)} \ldots = 0$.

Derivation of the BBGKY Hierarchy

- Back to the original equation:

$$\frac{\partial P^{(s)}}{\partial t} + \sum_{i=1}^{s} \xi_i \frac{\partial P^{(s)}}{\partial x_i} = (N-s) \sum_{i=1}^{s} \int P^{(s+1)} \cdot (\xi_i - \xi_{s+1}) \cdot n_i d\sigma_i d\xi_{s+1}$$

$$\overset{x_{s+1} \to x_i - n\sigma}{=} (N-s)\sigma^2 \sum_{i=1}^{s} \int_{S^2} P^{(s+1)} (\xi_i - \xi_{s+1}) \cdot n \, dn \, d\xi_{s+1}$$

$$=: Q^{\sigma}_{s+1} P^{(s+1)}(z^s, t)$$

- For less stringent assumptions, we obtain the general form of the Born-Bogoliubov-Green-Kirkwood-Yvon (BBGKY) hierarchy:

Theorem (BBGKY Hierarchy)

$$\begin{aligned} \frac{d}{dt} P^{(s)}(T^t z^s, t) &= Q^{\sigma}_{s+1} P^{(s+1)}(T^t z^s, t) \\ Q^{\sigma}_{s+1} P^{(s+1)}(T^t z^s, t) &= (N-s)\sigma^2 \sum_{i=1}^{s} \int dn \int d\xi_{s+1} (\xi_i - \xi_{s+1}) \cdot n \\ &\quad P^{(s+1)}(T^t z^s, T^t x_i - n\sigma, \xi_{s+1}, t) \end{aligned}$$

Outline

Informal Derivation of the Boltzmann Equation

- BBGKY hierarchy is impractical for real calculations: Equation for $P^{(s)}$ depends of $P^{(s+1)}$.
- Intuitively, chaotic particle motion should be uncorrelated
  $\Rightarrow$ There should be a closed equation for $P^{(1)}(x, \xi, t)$
- "Chaos" means

$$P^{(s)}(x_1, \xi_1 \ldots x_s, \xi_s, t) = \prod_{i=1}^{s} P^{(1)}(x_i, \xi_i, t)$$

- We will work in the Boltzmann-Grad Limit $N \to \infty$, $\sigma \to 0$, $N\sigma^2 = \alpha \in \mathbb{R}$.
- Insert this into the BBGKY equation for $P^{(1)}$:

$$\begin{aligned}
\frac{dP^{(1)}(x, \xi, t)}{dt} &= Q_2^{\sigma} P^{(2)}(x, \xi, t) \\
&= \alpha \int_{S^2} dn \int d\xi_* (\xi - \xi_*) \cdot n \, P^{(2)}(x, \xi, x, \xi_*, t) \\
&= \alpha \int_{(\xi - \xi_*) \cdot n > 0} dn \int d\xi_* |(\xi - \xi_*) \cdot n| \\
&\qquad \Big(P^{(1)}(x, \xi', t) P^{(1)}(x, \xi_*', t) - P^{(1)}(x, \xi, t) P^{(1)}(x, \xi_*, t) \Big)
\end{aligned}$$

Informal Derivation of the Boltzmann Equation

- We obtain the Boltzmann Equation:

$$\frac{dP^{(1)}(x,\xi,t)}{dt} = \alpha \int_{S^+} dn \int d\xi_* |(\xi - \xi_*) \cdot n| \Big(P^{(1)}(x,\xi',t) P^{(1)}(x,\xi'_*,t) - P^{(1)}(x,\xi,t) P^{(1)}(x,\xi_*,t) \Big)$$

- Intuitive illustration: Without collisions the Liouville equation yields

$$\frac{\partial P^{(1)}}{\partial t} + \xi \frac{\partial P^{(1)}}{\partial x} = 0$$

- The right hand side of the Boltzmann Equation has the form *Gain* $-$ *Loss* $\Rightarrow$ It describes the influence of collisions.
- The informal derivation lacks the proofs that
  - The chaos assumption $P^{(s)} = \prod P^{(1)}$ is justified for $t > 0$
  - The limit $N \to \infty$, $\sigma \to 0$, $N\sigma^2 = \alpha$ exists.

Formulation of the Theorem

- Start with the BBGKY hierarchy:

$$\begin{aligned} \frac{d}{dt} P^{(s)}(T^t z^s, t) &= Q^{\sigma}_{s+1} P^{(s+1)}(T^t z^s, t) \\ Q^{\sigma}_{s+1} P^{(s+1)}(T^t z^s, t) &= (N-s)\sigma^2 \sum_{i=1}^{s} \int_{S^2} dn \int d\xi_{s+1} (\xi_i - \xi_{s+1}) \cdot n \\ & \quad P^{(s+1)}(T^t z^s, T^t x_i - n\sigma, \xi_{s+1}, t) \end{aligned}$$

- In the Boltzmann-Grad limit $N \to \infty$, $\sigma \to 0$, $N\sigma^2 = \alpha$ we expect to obtain the Boltzmann Hierarchy

$$\frac{d}{dt} f^{(s)}(T_0^t z^s, t) = Q^0_{s+1} f^{(s+1)}(T_0^t z^s, t)$$

where T_0^t denotes collisionless flow.
- If $f^{(s)}(z^s, t) = \prod_{i=1}^{s} f(x_i, \xi_i, t)$, the Boltzmann hierarchy and the Boltzmann equation are equivalent.
- Idea: Prove that the Boltzmann hierarchy is really the limit of the BBGKY hierarchy and that its solution factorizes under certain assumptions.

Formulation of the Theorem

Theorem (Rigorous Validity of the Boltzmann Equation)

Let $(\Lambda \times \mathbb{R}^3)^{s,\sigma}_{\neq} = \left\{ z^s \in \Lambda^s \times \mathbb{R}^{3s}; |x_i - x_j| > \sigma, i \neq j, \sigma \geq 0 \right\}$. *Assume that*

1. $P_0^{(s)}(z^s) = P^{(s)}(z^s, 0)$ *is continuous on* $(\Lambda \times \mathbb{R}^3)^{s,\sigma}_{\neq}$ *and at collision points.*
2. *The limit* $\lim_{N\to\infty} P_0^{(s)} = f_0^{(s)}(z^s)$ *with continuous* $f_0^{(s)} : \Lambda^s \times \mathbb{R}^{3s} \to \mathbb{R}$ *exists and is uniform on compact subsets of* $(\Lambda \times \mathbb{R}^3)^{s,\sigma}_{\neq}$.
3. *The initial values satisfy* $f_0^{(s)}(z^s) = \prod_{i=1}^{s} f_0(x_i, \xi_i)$ *("Initial chaos")*
4. *There are positive constants* β, C *and* b *such that* $\sup_{z^s} P_0^{(s)} \leq C \cdot b^s \cdot \exp\left(-\beta \sum_{i=1}^{s} \xi_i^2\right)$

Then, on a sufficiently small interval $[0, t_0]$ *the solution of the Boltzmann hierarchy exists and is unique. It is the limit of the solution of the BBGKY hierarchy and has the form* $f^{(s)}(z^s, t) = \prod_{i=1}^{s} f(x_i, \xi_i, t)$, *i.e. factorization is preserved. Here* f *is a solution of the Boltzmann equation to the initial data* f_0.

(Full Proof: Cercignati, Illner, Pulvirenti: The Mathematical theory of Dilute Gases, Springer 1994)

Outline of the Proof

- The BBGKY hierarchy $\frac{d}{dt} P^{(s)}(T^t z^s, t) = Q^\sigma_{s+1} P^{(s+1)}(T^t z^s, t)$ is solved by

$$P^{(s)}(T^t z^s, t) = P_0^{(s)}(z^s) + \int_0^t dt_1 \left(Q^\sigma_{s+1} P^{s+1}\right)(T^{t_1} z^s, t_1)$$

$$\Leftrightarrow \; P^{(s)}(z^s, t) = S_\sigma(t) P_0^{(s)}(z^s) + \int_0^t dt_1 S_\sigma(t - t_1) \left(Q^\sigma_{s+1} P^{s+1}\right)(z^s, t_1)$$

  where $S_\sigma(t) f(z^s) = f(T^{-t} z^s)$.
- Iteration of this formula gives

$$P^{(s)}(z^s, t) = \sum_{n=0}^{N-s} \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n \; S_\sigma(t - t_1) Q^\sigma_{s+1} S_\sigma(t_1 - t_2) \ldots Q^\sigma_{s+n} S_\sigma(t_n) P_0^{(s+n)}(z^s)$$

- For the Boltzmann hierarchy:

$$f^{(s)}(z^s, t) = \sum_{n=0}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n \; S_0(t - t_1) Q^0_{s+1} S_0(t_1 - t_2) \ldots Q^0_{s+n} S_0(t_n) f_0^{(s+n)}(z^s)$$

  The series is infinite, therefore convergence is nontrivial!

Outline of the Proof

The proof proceeds as follows:

1. Show that the convergence of the BBGKY series $\sum a_n^\sigma$ to the Boltzmann series $\sum a_n^0$ holds term by term.
2. Find a series $\sum b_n < \infty$ satisfying $0 \leq |a_n^\sigma|, |a_n^0| \leq b_n$. The existence of such a series proves the convergence $\sum a_n^\sigma \to \sum a_n^0$.
3. Uniqueness follows from the constructions in the previous steps.
4. Proof of the factorization property:
   The solution of the Boltzmann hierarchy for $f^{(1)}$ exists according to step 1 and 2. Show that $f^{(s)} = \prod_{i=1}^s f^{(1)}(x_i, \xi_i, t)$ solves the Boltzmann hierarchy. By uniqueness (step 3) the propagation of chaos follows.

Some remarks on (ir)reversibility

- Consider the time reversal operation $\mathcal{T} : t \to -t$.
- Classical mechanics is invariant unter $\mathcal{T}$: Every motion can be reversed.
- The Boltzmann equation is not $\mathcal{T}$-invariant (no proof here):

$$\begin{array}{ccc} \dfrac{dP^{(1)}(x,\xi,t)}{dt} & = & \mathcal{C} \\ \big\downarrow \mathcal{T} & & \big\downarrow \mathcal{T} \\ -\dfrac{dP^{(1)}(x,\xi,t)}{dt} & = & \mathcal{C} \end{array}$$

- The proof of the Boltzmann equation shows how one can obtain irreversible dynamics from a reversible theory.
- Intuitive explanation: In Boltzmann dynamics, the inverse process requires initial conditions that are strongly disfavoured if initial chaos $f_0^{(s)} = \prod f$ holds.

Outline

Generalizations of the Boltzmann Equation

Electrons in a Metal

$$\frac{\partial f}{\partial t} + \frac{d\xi_i}{dt}\frac{\partial f}{\partial \xi_i} + \frac{dx_i}{dt}\frac{\partial f}{\partial x_i} = \frac{Vm^3}{(2\pi)^3}\int \Big[\underbrace{f(\xi')(1-f(\xi))\mathcal{S}(\xi' \to \xi)}_{\text{Gain}} - \underbrace{f(\xi)(1-f(\xi'))\mathcal{S}(\xi \to \xi')}_{\text{Loss}}\Big]$$

$f(x, \xi, t)$	= Electron distribution function	V	= Volume of the semiconductor
$\mathcal{S}$	= Scattering probability	m	= Electron mass

Particle Transport in the Early Universe

$$\frac{\partial n}{\partial t} + 3Hn = \mathcal{C}$$

$n(|x|, t)$ = Particle density, integrated over ξ

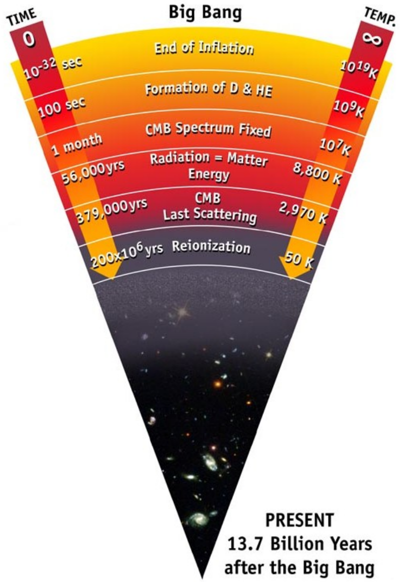
H = Hubble's constant parametrizing the expansion of the universe

$\mathcal{C}$ = Collision integral

Limitations of the Boltzmann Equation

Applicability of the Boltzmann Equation to processes in the early universe is doubtful:

- Time between two collisions is comparable to duration of collision
- Hard sphere potential is a bad approximation to the real dynamics
- Quantum Effects cannot be described by simple collision integrals



Conclusions

- The hard sphere model can describe many physical systems.
- Its microscopic evolution is governed by the Liouville equation $dP/dt = 0$.
- The BBGKY hierarchy connects the full probability density function P to the 1-particle distrbution $P^{(1)}$.
- In the Boltzmann-Grad limit $N \to \infty$, $\sigma \to 0$, $N\sigma^2 = \alpha$ we obtain the Boltzmann equation

$$\frac{dP^{(1)}(x,\xi,t)}{dt} = N\sigma^2 \int_{S^+} dn \int d\xi_* |(\xi - \xi_*) \cdot n| \Big(P^{(1)}(x,\xi',t) P^{(1)}(x,\xi'_*,t) - P^{(1)}(x,\xi,t) P^{(1)}(x,\xi_*,t) \Big)$$

  which is a closed equation for the 1-particle distribution.
- The proof of the Boltzmann equation shows how irreversible behaviour arises in nature.
- The Boltzmann equation can be extended to describe complex systems like semiconductors or the early universe. However, it has its limitations in extreme situations.